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14. ABSTRACT
Final technical report for James Freericks' ONR superconducting electronics grant for the period from 1999--2005. This work involved the development of computer modeling codes to describe Josephson junctions with barrier materials that are tuned close to the metal-insulator transition. The figure of merit can be determined as a function of different parameters, including the proximity to the metal-insulator transition, the thickness of the barrier, and the temperature. We discovered a simple phenomenological parameter, called the generalized Thouless energy, that is useful for characterizing and summarizing the Josephson junction properties; much behavior of these systems becomes universal when represented in terms of this Thouless energy. We also developed a nonequilibrium many-body formalism that can determine the response of these systems to large electric fields. Much of the computational work was carried out on DOD parallel machines from the HPCMO facilities.

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Theoretical modeling of Josephson junctions for digital electronics (Final Technical Report)

James K. Freericks
November, 29, 2005

Summary:
This is the final technical report for James Freericks' ONR superconducting electronics grant for the period from 1999--2005. This work involved the development of computer modeling codes to describe Josephson junctions with barrier materials that are tuned close to the metal-insulator transition. The figure of merit can be determined as a function of different parameters, including the proximity to the metal-insulator transition, the thickness of the barrier, and the temperature. We discovered a simple phenomenological parameter, called the generalized Thouless energy, that is useful for characterizing and summarizing the Josephson junction properties; much behavior of these systems becomes universal when represented in terms of this Thouless energy. We also developed a nonequilibrium many-body formalism that can determine the response of these systems to large electric fields. Much of the computational work was carried out on DOD parallel machines from the HPCMO facilities.

Summary of technical projects completed

A. Modeling of Josephson junctions.
The major technical project completed in this grant was the development of a computer modeling program that can describe the behavior of Josephson junctions with the barriers tuned to lie close to a metal-insulator transition. This regime is of interest for self-shunted high speed JJs that would be used for ultrafast digital electronics. The main experimental system that was being worked on was materials with Ta_xN barriers, where the material undergoes and MIT when x=0.6. Our approach was based on inhomogeneous dynamical mean field theory, which is a nonperturbative technique that can determine the many-body Green's functions and transport of multilayered nanostructures. We developed a series of calculations that can describe the superconducting state and the situation where the superconductor carries current due to a phase gradient placed over the superconducting leads. This allows for a calculation of the current density of the JJ. Next, we developed a real-frequency, normal-state code, that can calculate the conductivity matrix via a Kubo formula, from which the resistance-area product can be determined. The product of these two quantities yields the JJ figure of merit. We examined a number of different cases through our studies including: (i) tuning the barrier through a MIT by varying the Coulomb interaction; (ii) examining the effects of electronic charge reconstruction that can drive the junction into a superconductor-insulator-normal metal-insulator-superconductor (SINIS) structure; (iii) temperature dependence of the figure of merit, critical current density and resistance, when the barriers are close to the MIT; and (iv) more complicated systems like SNSNS junctions, and so on. A comprehensive review article on this work was also completed.

We next were interested in determining whether there was any universality in our results that could be practically used to help predict properties of junctions from simple measurements (perhaps even in the normal state). Motivated by quasiclassical calculations, where the Thouless energy plays a prominent role (the Thouless energy is a quantum mechanical energy derived from the average or typical time that an electron spends inside the barrier of the JJ and Planck's constant). In the quasiclassical case, there is a universal formula for the figure of merit as a function of the Thouless energy. When the Thouless energy is larger than the superconducting gap, the figure of merit is proportional to the gap, while in cases where the Thouless energy is smaller than the gap, it determines the figure of merit. We found that all of our metallic barriers, no matter how strong the scattering, fit the quasiclassical curve perfectly. When we went through the MIT, we found a simple way to generalize the Thouless energy definition, and found the generalized result also fit closely to the quasiclassical curve, although the actual figure of merit was somewhat higher in the region where the Thouless energy determined the figure of merit. We feel this work can be employed both for diagnostic and design purposes of junctions. To get the best figure of merit, one wants to keep the Thouless energy larger than the superconducting gap, if at all possible.

B. Nonequilibrium physics

We also spent a significant effort on developing a many-body formalism to describe nonequilibrium physics. This allows for an understanding of the nonlinear response of a circuit element to large electric fields that could result from electronic warfare, or natural sources like lightning. Also, since nonlinearities often determine the limit of how "hard" a device can be pushed within its design specs, this theory also allows for an understanding of how devices fail under ordinary operating conditions. The nonequilibrium formalism was developed in the late 1950s and early 1960s, but to date there has not been any exact solution of the formalism for any strongly interacting system. Instead, much work has focused on perturbative effects, which may not be valid if the interactions are strong enough. We found a way to modify equilibrium dynamical mean field theory to work in the nonequilibrium case as well, and have studied two of the simplest problems with these techniques. The first problem is a "toy" problem that involves determining an equilibrium Green's function from the nonequilibrium approach, because there is no straightforward way to directly perform the analytic continuation to the real frequency axis. By carefully controlling the calculations, via exact sum rules, we were able to quantify how accurate the calculations were, and areas where the computational procedure can run into difficulties. Armed with these results, we next tackled the simplest nonequilibrium problem---the nonlinear response of a strongly correlated material to a large electric field. In a periodic system, the noninteracting response involves the so-called Bloch oscillations (similar in many respects to the finite voltage response of a JJ, where a dc voltage creates an ac current). As we turn interactions on, we can study how the Bloch oscillations decay. Although a simple Boltzmann equation approach indicates that the Bloch oscillations disappear immediately after scattering is turned on, our data indicates that the oscillations can be long lived, and maybe even survive in the steady state if the field is large enough.

C. Other miscellaneous work

During the grant period two comprehensive review articles were finished. One which summarized how to use inhomogeneous dynamical mean field theory to optimize the performance of a JJ with barriers tuned to lie close to the MIT, and the other which summarized over a decade worth of work on DMFT with a focus on the Falicov-Kimball model. In addition, a book is being written on the theory of multilayered nanostructures, including JJs and should be complete in March of 2006, with publication in the winter of 2006-07.

Other work included development of theories for stripe formation and phase separation due to strong electron-electron interactions. We were able to show under what conditions phase separation or stripe formation occurs. This is of interest in the high-temperature superconductor materials which may have stripe formation playing a role in the materials properties. We investigated spintronics, by developing a direct approach to disordered problems that includes the spin-orbit interaction and can describe the Rashba coupling. We also spent a significant amount of time on thermal transport properties in the hopes of finding insight into how to develop low temperature thermoelectrics. We found some promising results from our theory when one is close to particle-hole symmetry, but has strong correlations, where the thermoelectric figure of merit can get large, But this region requires fine-tuning of parameters, and may be difficult to attain in real systems. We found more promising results at high temperature, where generically power generation appeared to be viable in many strongly correlated systems.

Relevance to the Superconducting Electronics program

The goal of this work was to provide a theoretical framework to help guide experimental design principles for optimized JJ performance. Finding a new technology for JJ digital electronics that will be adopted by foundries is not an easy task, and it requires a dramatic improvement of performance with limited extra complication in the processing of chips. Our work has not found the resolution for this problem to yield the newest JJ for digital electronics chips. Nevertheless, our work has shown a number of important principles, which include (i) when the barrier is on the metallic side of the MIT, then the temperature dependence of the figure of merit is the most important quantity for determining whether circuits can be made. Variations in the critical current as a function of temperature were quite detrimental for the Ta_xN-based junctions and our theory indicated that this is an intrinsic problem, that will not be easily overcome, but perhaps could be addressed by making the barriers more insulating. (ii) We devised a new metric, based on a generalized Thouless energy, to use in determining how well a device will function. Since the Thouless energy can be determined in the normal state, it provides a simpler diagnostic than other metrics, but it has not yet been adopted by experimentalists. Finally, we worked on developing a new formalism that can shed light on nonlinear effects in many different kinds of devices, and will likely find wide use as more devices with strongly correlated materials are made.

Personnel supported:

This grant supported one postdoctoral fellow per year: Paul Miller (1999, now at Brandeis University), Branislav Nikolic (2000—2002, now assistant professor at the University of Delaware), Veljko Zlatic and Serhii Shafraniuk (2002--2003), and Alireza Tahvildar-Zadeh (2003—2005). In addition, a graduate student, Alexander Joura, was supported in 2002—2003. The PI was partially supported during the summer months.

Publications during the grant period

[1] J. K. Freericks and R. Lemanski, Segregation and charge-density-wave order in the spinless Falicov-Kimball model, Phys. Rev. B **61** 13438--13444 (2000).

[2] J. K. Freericks and P. Miller, Dynamical charge susceptibility of the spinless Falicov-Kimball model, Phys. Rev. B **62**, 10022--10032 (2000).

[3] P. Miller and J. K. Freericks, Microscopic self-consistent theory of Josephson junctions including dynamical electron correlations, J. Phys.: Conden. Mat. **13,** 3187--3213 (2001).

[4] Ch. Gruber, N. Macris, Ph. Royer, and J. K. Freericks, Higher period ordered phases on the Bethe lattice, Phys. Rev. B. **63**, 165111-1--11 (2001).

[5] J. K. Freericks, B. K. Nikolic, and P. Miller, Tuning a Josephson junction through a quantum critical point, Phys. Rev. B **64,** 054511 (2001); Erratum: Phys. Rev. B **68**, 099901 (2003).

[6] B. K. Nikolic, J. K. Freericks, and P. Miller, Equilibrium properties of double-screened-dipole-barrier SINIS Josephson junctions, Phys. Rev. B **65**, 064529-1--11 (2002); Virtual Journal of Applications of Superconductivity, Vol. **2**, Iss. **3**.

[7] B. K. Nikolic, J. K. Freericks, and P. Miller, Suppression of the ``quasiclassical" proximity gap in correlated-metal--superconductor structures, Phys. Rev. Lett. **88**, 077002-1--4 (2002); Virtual Journal of Nanoscale Science & Technology, Vol. **5**, Iss. **7**.

[8] J. K. Freericks, E. H. Lieb, and D. Ueltschi, Segregation in the Falicov-Kimball model, Commun. Math. Phys. **227**, 243--279 (2002).

[9] B. K. Nikolic, J. K. Freericks, and P. Miller, Reduction of Josephson critical current in short ballistic SNS weak links, Phys. Rev. B **64,** 212507--1-4 (2001).

[10] J. K. Freericks, B. K. Nikolic, and P. Miller, Optimizing the speed of a Josephson junction with dynamical mean-field theory, Int. J. Mod. Phys. B **16**, 531--561 (2002).

[11] J. K. Freericks, E. H. Lieb, and D. Ueltschi, Phase separation due to quantum mechanical correlations, Phys. Rev. Lett. **88,** 106401--1-4 (2002). [Reprinted in

Condensed Matter Physics and Exactly Soluble Models: Selecta of Elliott H. Lieb, Edited by B. Nachtergaele, J. P. Solovej, and J. Yngvason (Springer, Berlin, 2004), pp. 119--122].

[12] J. K. Freericks, B. K. Nikolic, and P. Miller, Temperature dependence of Superconductor-Correlated Metal-Superconductor Josephson junctions, Appl. Phys. Lett. **82**, 970--972 (2003); Virtual Journal of Applications of Superconductivity, **4**, Issue 4 (2003). Erratum: Appl. Phys. Lett. **83**, 1275 (2003).
[13] J. K. Freericks, D. Demchenko, A. Joura, and V. Zlatic', Optimizing thermal transport in the Falicov-Kimball model: binary-alloy picture, Phys. Rev. B **68**, 195120--1-12 (2003).

[14] J. K. Freericks and V. Zlatic', Exact dynamical mean field theory of the Falicov-Kimball model, Rev. Mod. Phys. **75**, 1333--1382 (2003).

[15] J. K. Freericks and V. Zlatic', Application of the multicomponent Falicov-Kimball model to intermediate-valence materials: $YbInCu_4$ and $EuNi_2(Si_{1-x}Ge_x)_2$, (Proceedings of the Physics of Magnetism, Poznan, Poland), physica status solidi (b) **236**, 265--271 (2003).

[16] B. K. Nikolic and J. K. Freericks, Mesoscopic spintronics: Fluctuation and localization effects in spin-polarized quantum transport, *Toward the controllable quantum states*, edited by H. Takayanagi and J. Nitta (World Scientific, 2003).

[17] J. K. Freericks, B. K. Nikolic, and P. Miller, Superconductor-Correlated Metal-Superconductor Josephson junctions: an optimized class for high speed digital electronics, (Proceedings of the Applied Superconductivity Conference, Houston, Texas) IEEE Trans. Appl. Supercond. **13**, 1089--1092 (2003).

[18] J. K. Freericks, Crossover from tunneling to incoherent (bulk) transport in a correlated nanostructure, Appl. Phys. Lett. **84**, 1383--1385 (2004); Virtual Journal of Nanoscale Science and Technology, **9**, Issue 8 (2004); Virtual Journal of Applications of Superconductivity, **6**, Issue 5 (2004).

[19] A. V. Joura, D. O. Demchencko, and J. K. Freericks, Thermal transport in the Falicov-Kimball model on a Bethe lattice, Phys. Rev. B **69**, 165105--1-5 (2004).

[20] D. O. Demchencko, A. V. Joura, and J. K. Freericks, Effect of particle-hole asymmetry on the Mott-Hubbard metal-insulator transition Phys. Rev. Lett. **92**, 216401--1-4 (2004).

[21] J. K. Freericks, V. M. Turkowski, and V. Zlatic', F-electron spectral function of the Falicov-Kimball model in infinite dimensions: The half-filled case, Phys. Rev. B **71**, 115111--1-12 (2005).

[22] J. K. Freericks, Dynamical mean field theory for strongly correlated inhomogeneous multilayered nanostructures, Phys. Rev. B **70**, 195342--1-14 (2004).

[23] V. M. Turkowski and J. K. Freericks, Nonlinear response of Bloch electrons in infinite dimensions, Phys. Rev. B **71**, 085104--1-11 (2005).

[24] J. K. Freericks, V. M. Turkowski, and V. Zlatic', F-electron spectral function near a quantum critical point, (proceedings of the Strongly Correlated Electron Systems conference, Karlsruhe, Germany), Physica B **359--361C**, 684--686 (2005).

[25] J. K. Freericks, V. M. Turkowski, and V. Zlatic', Parallelizing the Keldysh formalism for strongly correlated electrons, in *Proceedings of the Users Group Conference Williamsburg, VA, June 7--11, 2004* (IEEE Computer Society, Los Alamitos, CA, 2004), p. 7--16.

[26] J. K. Freericks, Strongly correlated multilayered nanostructures near the Mott transition, (proceedings of the 24th international conference in theoretical physics, Ustron, Poland, 2004) phys. stat. sol. b **242**, 189--195 (2005).

[27] J. K. Freericks, A. N. Tahvildar-Zadeh, and B. K. Nikolic, Use of a generalized Thouless energy in describing transport properties of Josephson junctions, (proceedings of the Applied Superconductivity Conference, Jacksonville, FL, 2004) IEEE Trans. Appl. Supercond. **15**, 896--899 (2005).

[28] J. K. Freericks, A. N. Tahvildar-Zadeh, and B. K. Nikolic, Thouless energy of strongly correlated electrons, *submitted to* Phys. Rev. B.

[29] J. K. Freericks, V. M. Turkowski, and V. Zlatic', Real-time formalism for studying the nonlinear response of "smart" materials to an electric field, in *Proceedings of the Users Group Conference Nashville, TN, June 28--30, 2005* (IEEE Computer Society, Los Alamitos, CA, 2005), submitted.

Invited talks

(Institutions)

[1] ``*Ultrafast digital electronics: optimizing the speed of a Josephson-junction,"* presented at the Ohio State University, The Newton Institute (Cambridge), University of Bristol, Institute of Low-Temperature and Structure Research, Wroclaw, Poland, Northwestern University, IBM, Almaden, and Conductus (2000-01).

[2] ``*Higher-period ordered phases on the Bethe lattice,"* presented at Princeton University (2001).

[3] ``*Superconductor-Correlated Metal-Superconductor Josephson junctions: a new class of junctions for optimal switching speed*" presented at the Institute of Magnetism, Kiev, Ukraine (June, 2002).

[4] ``*A simplified explanation of the Mott insulator-superfluid transition in the Bose Hubbard model*", National Institute of Standards and Technology, Gaithersberg (November, 2002).

[5] ``*Crossover from tunneling to Ohmic transport in junctions close to the metal-insulator transition*", IBM Almaden Research Center (October, 2003).

(Conferences)

[1] ``*Nonlinear response of a Mott insulator*", Dynamical Mean-Field Theory for Correlated Electrons: Applications to Real Materials, Extensions and Perspectives Workshop, International Center for Theoretical Physics, Trieste, Italy (August, 2005).

[2] ``*Optimizing Josephson junction performance and nonlinear effects in "smart" electronics*", Office of Naval Research Superconducting Electronics Program Review, Red Bank, NJ (February, 2005).

[3] ``*Strongly correlated multilayered nanostructures near the Mott transition*" 28th International conference on nano and macro systems, Ustron, Poland (September, 2004).

[4] ``*Modeling Josephson junctions with correlated metal barriers,*" Office of Naval Research Superconducting Electronics Program Review, Melbourne, FL (February, 2003).

[5] ``*Theoretical description of the high-temperature phase of Yb and Eu intermetallics*" Physics of Magnetism Conference, Poznan, Poland (June, 2002).

[6] ``*Modeling Josephson junctions near the metal-insulator transition*", Office of Naval Research superconducting electronic program review, Lake Estes, Colorado (February, 2002).

[7] ``*Modeling Schottky barrier SINIS junctions,*" and ``*Tuning a Josephson junction through a metal-insulator transition*", Office of Naval Research superconducting electronic program review, Sedona, Arizona (February, 2001).

[8] ``*Modeling of Josephson junctions with charge redistribution at the interface,*" Workshop on grain boundaries and interfaces in high-temperature superconductors (Satellite conference of the Applied Superconductivity Conference) sponsored by the University of Wisconsin Grain Boundary Group (September, 2000).

[9] ``*Self-consistent modeling of SINIS and SNSNS Josephson junctions,*'' Workshop on SINIS junctions, (Satellite conference of the Applied Superconductivity Conference) (September, 2000).

[10] ``*Ultrafast digital electronics: optimizing the speed of a Josephson-junction,*'' Office of Naval Research, Superconducting Electronics Program Review, Cape Cod, MA (March, 2000).

[11] ``*Modeling the anomalous thermodynamic and transport properties of Ytterbium intermetallic compounds,*'' Concepts in Electron Correlations, Hvar, Croatia (September, 1999).

[12] ``*A microscopic model of the Josephson-junction interface,*'' Office of Naval Research, Superconducting Electronics Workshop, Bakersfield, CA (January, 1999).